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Electronic and impurity states in a three-dimensional corner under an applied electric field

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Abstract. We study the electronic and impurity states in a three-dimensional corner under an applied electric field. It is found that the electronic states in the corner are discrete in all three directions, similar to the electronic state behaviour in a quantum dot, and the eigenenergies of the discrete electronic levels increase with the electric field strength. The impurity states in the three-dimensional corner have similar features as those in the quantum dots, and their maximum binding energy increases, but the impurity position corresponding to the peak binding energy moves towards the corner, as the electric field strength increases. The results also show that the binding energy of the ground impurity state at the corner point in the absence of electric field is equal to that of the fourth impurity excited state in the bulk.

1. Introduction

The advances in microfabrication techniques, such as molecular beam epitaxy (MBE) and metal–organic chemical vapour deposition (MOCVD), make it possible to confine electrons in one, two or all three directions (quantum wells, wires and dots). The interfaces in these low-dimensional systems play a significant role in determining their electronic and optical properties, and step structures usually exist at the interfaces [1–7], which affect their optical transition spectra considerably. In fact, a stepped surface or V-shaped groove of large size in an interface can be viewed as a corner. This model has been adopted by Lee and Antoniewicz [8, 9] in studying the surface bound states and surface polaron states.

In our previous papers [10–13], we have studied the electronic and impurity states in a two-dimensional corner with and without an applied electric field, and many interesting results were obtained. For example, it was found that the ground impurity binding energy in the absence of electric field is equal to that of the third impurity excited state in the bulk when the impurity is placed at the corner point [10], and the electronic and impurity states in the corner under an applied electric field are similar to those in quantum wires [13]. In the present paper, we study the electronic and impurity states in a three-dimensional corner under an applied electric field. Because of the existence of the external electric field, the electrons are pushed towards the corner and the motion of electrons in the corner is confined in all three directions, analogous to that in a quantum dot. It is expected that the electronic and impurity state behaviour in the three-dimensional corner under the externally applied electric field is similar to that in quantum dots. In section 2, the electronic states are analysed. In section 3, the impurity binding energies are calculated with the use of the variational method. The numerical results and discussion are given in section 4.

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2. Electronic states

Let us consider an electron moving in a three-dimensional corner structure with the well material inside the corner and barrier material outside the corner, and an electric field $\boldsymbol{F} = (1, 1, 1)(F/\sqrt{3})$ is applied along the diagonal line of the corner. In the effective-mass approximation, the Hamiltonian for electron states in the corner can be written

$$H^{(0)}(\boldsymbol{r}) = \frac{\boldsymbol{P}^2}{2m_b} + eFx/\sqrt{3} + eFy/\sqrt{3} + eFz/\sqrt{3} + V(\boldsymbol{r}) \tag{1}$$

where m_b is the electron-band effective mass and $\boldsymbol{r}$ and $\boldsymbol{P}$ are the electron coordinate and momentum, respectively. The electron-confining potential well in the corner is given by

$$V(\boldsymbol{r}) = \begin{cases} 0 & x > 0,\ y > 0 \text{ and } z > 0 \\ \infty & \text{otherwise.} \end{cases} \tag{2}$$

2.1. $F = 0$

In the absence of electric field, the electron energy levels in the corner are continuous. As the simplest approximation [10], the electronic wavefunction for the Hamiltonian $H^{(0)}(\boldsymbol{r})$ can be written

$$\Phi(\boldsymbol{r}) = N_0 \sin(k_x x) \sin(k_y y) \sin(k_z z) \tag{3}$$

where N_0 is the normalization constant and the electron energy is given by

$$E = \frac{\overline{h}^2}{2m_b}(k_x^2 + k_y^2 + k_z^2). \tag{4}$$

The ground-state wavefunction and energy level are

$$\Phi_0(\boldsymbol{r}) = 0 \tag{5a}$$

$$E_0 = 0. \tag{5b}$$

2.2. $F > 0$

When the electric field is added, as the variables can be separable [13], the electronic wavefunction for Hamiltonian $H^{(0)}(\boldsymbol{r})$ is written

$$\begin{aligned} &\Phi(\boldsymbol{r}) = N_0 Ai(\xi) Ai(\eta) Ai(\zeta) \\ &\xi = (x/l) - \lambda_l \\ &\eta = (y/l) - \lambda_m \\ &\zeta = (z/l) - \lambda_n \\ &l = [\sqrt{3}\overline{h}^2/(2m_b eF)]^{1/3} \end{aligned} \tag{6}$$

where l is the electron characteristic length under the electric field, λ_l, λ_m and λ_n are the dimensionless constants, and $Ai(\xi)$ is the Airy function which is defined by [14]

$$Ai(\xi) = \begin{cases} \frac{1}{3}\sqrt{|\xi|}[J_{1/3}(\frac{2}{3}|\xi|^{3/2}) + J_{-1/3}(\frac{2}{3}|\xi|^{3/2})] & \xi < 0 \\ (1/\pi)\sqrt{\xi/3}K_{1/3}(\frac{2}{3}|\xi|^{3/2}) & \xi > 0 \end{cases} \tag{7}$$

where $J_{1/3}$ is the Bessel function with order 1/3, and $K_{1/3}$ is the modified Bessel function of the second kind with order 1/3. The electronic wavefunction $\Phi(\boldsymbol{r})$ satisfies the following boundary conditions

$$\Phi(\boldsymbol{r})|_{x=0} = \Phi(\boldsymbol{r})|_{y=0} = \Phi(\boldsymbol{r})|_{z=0} = 0 \tag{8a}$$

which are equivalent to

$$Ai(-\lambda_l) = Ai(-\lambda_m) = Ai(-\lambda_n) = 0 \tag{8b}$$

where l, m, $n = 1, 2, 3, \ldots$ are positive integers, $\lambda_{l(m,n)}$ is the zero point of the Airy function, and $\lambda_1 = 2.338\,11$, $\lambda_2 = 3.271\,09$, $\lambda_3 = 5.520\,56, \ldots$. The electron energy levels are given by

$$E_{lmn} = \frac{\overline{h}^2}{2m_b l^2}(\lambda_l + \lambda_m + \lambda_n). \tag{9}$$

The electronic wavefunction in the ground state is

$$\begin{aligned} &\Phi_0(\boldsymbol{r}) = N_0 Ai(\xi) Ai(\eta) Ai(\zeta) \\ &\xi = (x/l) - \lambda_1 \\ &\eta = (y/l) - \lambda_1 \\ &\zeta = (z/l) - \lambda_1 \end{aligned} \tag{10}$$

and the electron energy in the ground state is

$$E_0 = 3\overline{h}^2\lambda_1/(2m_b l^2). \tag{11}$$

3. Impurity states

When the impurity is placed at the position $\boldsymbol{r}_0 = (x_0, y_0, z_0)$ inside the corner, the Hamiltonian for impurity states can be written

$$H(\boldsymbol{r}) = \frac{\boldsymbol{P}^2}{2m_b} + eFx/\sqrt{3} + eFy/\sqrt{3} + eFz/\sqrt{3} + V_{ion}(\boldsymbol{r}) + V(\boldsymbol{r}) \tag{12}$$

where

$$V_{ion}(\boldsymbol{r}) = -e^2/(\varepsilon|\boldsymbol{r} - \boldsymbol{r}_0|) \tag{13}$$

and ε is the dielectric constant of the well material.

From equation (3), we can see that the first term of the expansion series of the electronic wavefunction in the absence of electric field is proportional to xyz when x, y and z are small. As in the case of quantum wells [15] and quantum wires [16] and in the light of the above analyses on electronic wavefunctions in the corner, we construct the following trial wavefunction for the ground impurity state

$$\psi(\boldsymbol{r}) = N(\beta)xyz\exp(-\beta|\boldsymbol{r} - \boldsymbol{r}_0|) \qquad \text{for } F = 0 \tag{14}$$

and

$$\begin{aligned} &\psi(\boldsymbol{r}) = N(\beta)Ai(\xi)Ai(\eta)Ai(\zeta)\exp(-\beta|\boldsymbol{r} - \boldsymbol{r}_0|) \\ &\xi = (x/l) - \lambda_1 \qquad \text{for } F > 0 \\ &\eta = (y/l) - \lambda_1 \\ &\zeta = (z/l) - \lambda_1 \end{aligned} \tag{15}$$

where $N(\beta)$ is the normalization constant, β is the variational parameter. The above trial wavefunction satisfies the boundary conditions.

As usual, the impurity binding energy E_b is defined as the energy difference between the bottom of the electronic conduction band without the impurity and the ground-state energy level of impurity states in the corner

$$E_b = E_0 - \min_{\beta} \langle \psi(\boldsymbol{r}) | H(\boldsymbol{r}) | \psi(\boldsymbol{r}) \rangle. \tag{16}$$

The above integral was calculated numerically.

4. Results and discussion

As an example, we choose AlAs/GaAs for numerical calculations [10] with GaAs being the well material and AlAs being the barrier material. For simplicity, the energy is in units of effective Rydbergs, $\mathrm{Ryd}^* = m_b e^4/(2\bar{h}^2\varepsilon^2)$, and the length is normalized to the effective Bohr radius $a_0^* = \bar{h}^2\varepsilon/(m_b e^2)$.

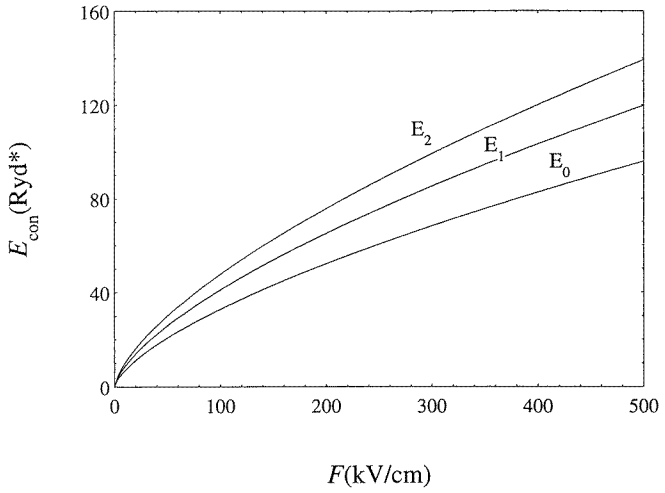

Figure 1. The electron confined energy levels versus the applied electric field in a three-dimensional corner. E_0, E_1 and E_2 represent the electron confined energy levels of the ground state, the first excited state and the second excited state, respectively.

The dependence of the electron confined energy levels on the applied electric field in a three-dimensional corner is shown in figure 1, which indicates that the electron energy levels increase with the electric field strength. Because of the existence of the electric field, the electrons are confined in all three directions in the corner, which is similar to the case where the electrons are confined in a quantum dot. We define the equivalent sizes of quantum dots in such a way that the ground electron energy level in the three-dimensional corner is equal to that in a cubic quantum box or a spherical quantum dot as follows

$$\frac{\bar{h}^2}{2m_b l^2} 3\lambda_1 = \frac{\bar{h}^2}{2m_b} \frac{3\pi^2}{L_{eq}^2} \qquad \text{for a cubic quantum box}$$

$$\frac{\bar{h}^2}{2m_b l^2} 3\lambda_1 = \frac{\bar{h}^2}{2m_b} \frac{4\pi^2}{D_{eq}^2} \qquad \text{for a spherical quantum dot}$$

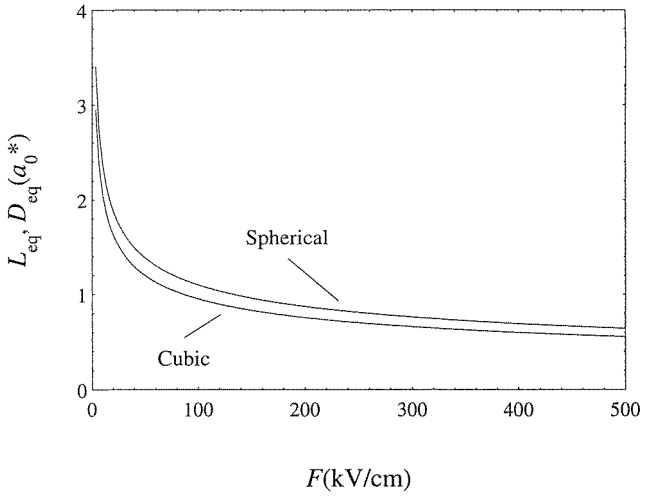

Figure 2. The equivalent sizes of quantum dots versus the applied electric field for the case where the ground electronic level in the three-dimensional corner is equal to that in the quantum dots. L_{eq} and D_{eq} represent the equivalent side width of a cubic quantum box and the equivalent diameter of a spherical quantum dot, respectively.

where L_{eq} is the equivalent side width of the cubic quantum box [17, 18] and D_{eq} is the equivalent diameter of the spherical quantum dot [19–23]. Figure 2 shows the relationship between the equivalent sizes of quantum dots and the applied electric field strength. The results of figure 2 indicate that, with increasing electric field strength, the equivalent sizes of quantum dots decrease, indicating stronger confinement on electrons in the corner under the stronger electric field. Moreover, the equivalent size of the cubic quantum box is smaller than that of the spherical quantum dot for the same electric field strength, which is due to the fact that the volume of the cubic box is larger than that of the spherical dot when the side width (L_{eq}) of the cubic quantum box is equal to the diameter (D_{eq}) of the spherical quantum dot, because the confinement of electrons in a quantum dot is related only to the quantum dot volume [18].

Figure 3 shows the dependence of the impurity binding energy on the impurity position along the diagonal line of the three-dimensional corner for three different electric fields. In the absence of electric field, we found that the impurity binding energy at the corner point ($x_0 = y_0 = z_0 = 0$) is 0.0625 Ryd*, which is equal to the value of the fourth impurity excited state in the bulk (1/16 Ryd*). From figure 3, it can be also seen that, when the electric field is not applied ($F = 0$), with increasing distance of the impurity away from the corner, the impurity binding energy increases gradually, and finally tends to the value 1 Ryd* in the bulk; however, when the electric field is applied, with increasing distance of the impurity away from the corner, the impurity binding energy increases at first, then reaches a peak value, and finally decreases monotonically. Moreover, as the electric field strength increases, the peak impurity binding energy becomes larger, and the impurity position corresponding to the peak value is closer to the corner point. These results are consistent with the variations in impurity binding energy with the sizes of quantum dots [17–23]. Figure 4 shows the dependence of the impurity binding energy on the impurity position along one corner line for different electric fields. The variations in impurity binding energy with the impurity position in figure 4 are similar to those in figure 3, except that the

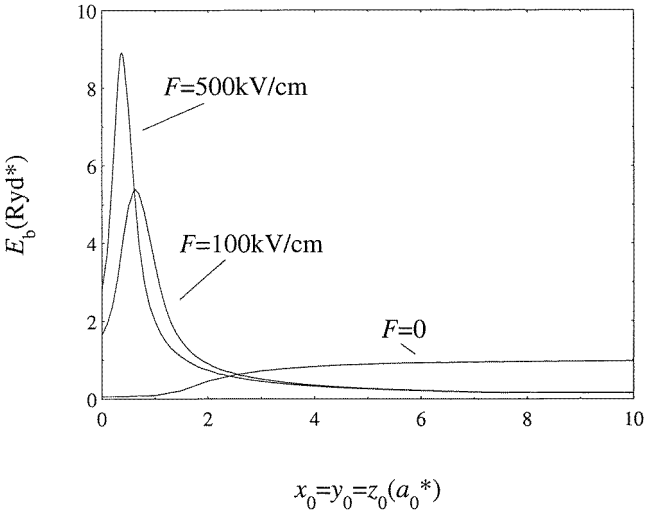

Figure 3. The ground impurity binding energy versus the impurity position along the diagonal line of the three-dimensional corner for three different electric fields.

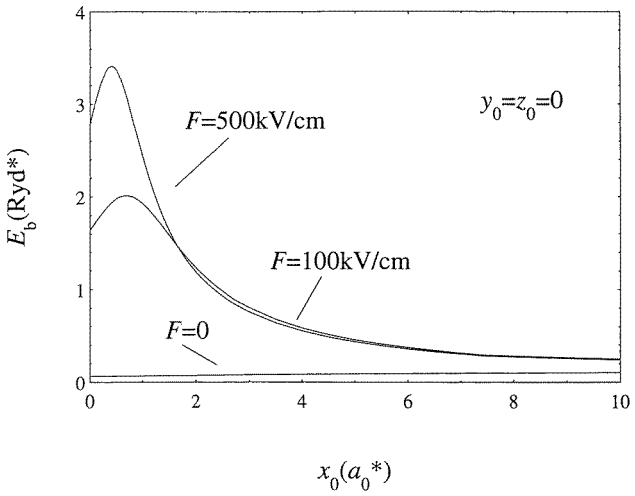

Figure 4. The ground impurity binding energy versus the impurity position along one corner line of the three-dimensional corner for three different electric fields.

impurity binding energies along the corner line are smaller than those along the diagonal line. In addition, when the electric field is absent and the impurity position is far away from the corner point, the impurity binding energy along one corner line is equal to the value (1/9 Ryd*) of the third impurity excited state in the bulk [10, 13].

Figure 5 shows the dependence of the impurity binding energy in the three-dimensional corner on the electric field strength for three different impurity positions. The results in figure 5 indicate that, when the impurity is at the corner point ($x_0 = y_0 = z_0 = 0$), with increasing electric field strength, the impurity binding energy increases monotonically; however, when the impurity is away from the corner point, the impurity binding energy

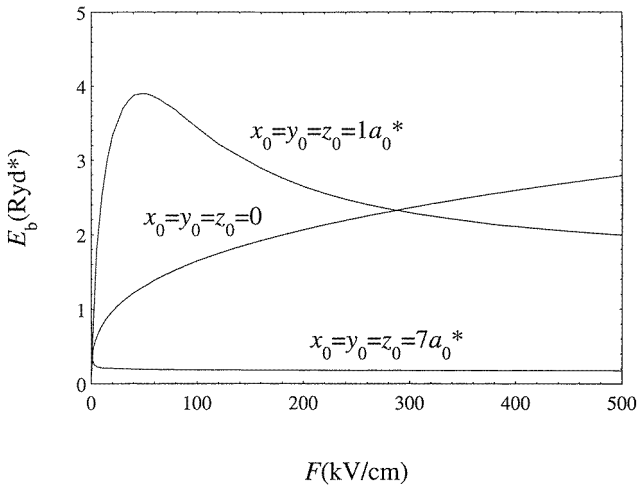

Figure 5. The ground impurity binding energy in a three-dimensional corner versus the electric field strength for three different impurity positions.

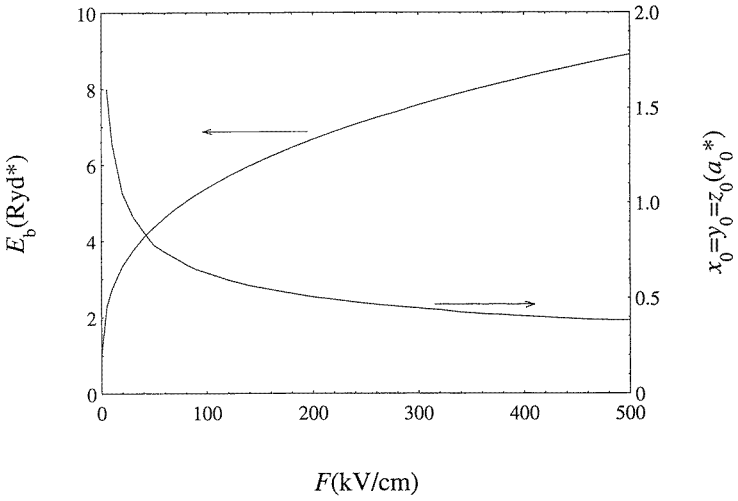

Figure 6. The maximum impurity binding energy and its corresponding impurity position in a three-dimensional corner versus the electric field strength.

increases at first, then reaches a peak value and finally decreases monotonically. Moreover, when the impurity is far away from the corner point, such as $x_0 = y_0 = z_0 = 7a_0^*$, with increasing electric field strength, the impurity binding energy almost decreases monotonically, as the peak point is very close to the corner point. The above results also tell us that there is a maximum impurity binding energy in the corner for a fixed electric field. Figure 6 shows the dependence of the peak impurity binding energy and its corresponding impurity position in a three-dimensional corner on the electric field strength, which indicates that the peak impurity binding energy increases and its corresponding impurity position moves towards the corner point as the electric field strength increases.

The results obtained above are interesting and their physical interpretation and discussion are as follows. Because the electric field pushes the electrons towards the corner, the electrons in the well material are confined in all three directions in the three-dimensional corner and the electron energy in the corner is quantized completely, like the electrons confined in a quantum dot. As the electric field strength increases, the confinement of the electrons in the corner is strengthened, and the electron energy levels in the corner increase, as shown in figure 1. As we know, the electron energy levels in a quantum dot increase with decrease in its dimensions [17–23], and the equivalent sizes of quantum dots for the three-dimensional corner under an applied electric field decrease with increase in the electric field strength, as shown in figure 2. The impurity behaviour in the three-dimensional corner under the applied electric field is also like that in a quantum dot, due to the confinement of electrons in the corner. When the impurity is at the corner ($x_0 = y_0 = z_0 = 0$), it is equivalent to an impurity located at one corner point of a quantum box, and the impurity binding energy increases monotonically with the increase in the electric field strength, like the case where the impurity binding energy at one corner point of a quantum box increases monotonically with the decrease in its dimension [18]. When the impurity is not at the corner point, such as when the impurity position is at $x_0 = y_0 = z_0 = 1$ and $x_0 = y_0 = z_0 = 7a_0^*$ as shown in figure 5, the relative position of the impurity with respect to the centre of the equivalent dot can be moved by changing the electric field strength, that is, the relative impurity position can be changed through the centre of the equivalent dot by increasing the electric field strength. It is well known that the impurity at the centre of quantum dots has a maximum binding energy [17–23]; that the impurity binding energy increases at first, then reaches a peak value and finally decreases monotonically for the impurity position not at the corner point, as shown in figure 5, is a result of the variations in distance between the impurity and the centre of equivalent dot with the electric field strength. When the electric field strength is fixed, this means that the equivalent size of quantum dot is fixed. As the impurity position is changed from the corner point, then to the centre of the equivalent quantum box and finally away from the quantum box, the impurity binding energy increases at first, then reaches a peak value and finally decreases monotonically, as shown in figures 3 and 4. That the maximum impurity binding energy increases and its corresponding impurity position moves towards the corner point as the electric field strength increases, as shown in figure 6, is also in agreement with the results that the impurity binding energy at the centre of a quantum dot increases with decreases in its dimension [17–23]. Moreover, we found that the trial wavefunction for the ground impurity state in the corner point ($x_0 = y_0 = z_0 = 0$) in the absence of electric field, as shown in equation (14), is a combination of the wavefunctions of the fourth impurity excited state in the bulk if the variational parameter β is equal to $1/4$, that is

$$\psi(\boldsymbol{r}) = (c/2\,\mathrm{i})[\Psi_{4,3,2}(r,\theta,\varphi) - \Psi_{4,3,-2}(r,\theta,\varphi)]$$

where c is a constant and $\Psi_{nlm}(r,\theta,\varphi) = R_{nl}(r)Y_{lm}(\theta,\varphi)$ is the eigenfunction of the hydrogen atom [14]; so the ground impurity binding energy at the corner point without electric field is equal to the value ($1/16$ Ryd*) corresponding to the fourth impurity excited state in the bulk.

In summary, we have investigated the electronic and hydrogenic impurity states in a three-dimensional corner under an applied electric field, and the Airy function was adopted to deal with the electronic states, while a variational approach was used to treat the impurity states. It was found that the electron and impurity state behaviour in the three-dimensional corner under the applied electric field is similar to that in quantum dots. The results also showed that the ground impurity binding energy at the corner point in the absence of electric

field is equal to that of the fourth impurity excited state in the bulk. As we know, it is easier to fabricate a three-dimensional corner structure than to fabricate a quantum dot in experiments, and our theoretical results may provide a new way to detect and apply the quantum confining effects of quantum dots.

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